ARKIV FÖR FYSIK Band 11 nr 39

Communicated 11 April 1956 by ERIK HULTHÉN and GUSTAF ISING

Indicating of wave-numbers in spectrophotometric recording at high resolution

By BJÖRN-ÅKE KRANTZ and NILS ÅSLUND

With 14 figures in the text

Summary

In a previous publication [1] the authors have described a method for the indication of wave-number marks at constant intervals on a graphic recording of a spectrum. In the present paper an account is given of the development of the method for application to the precision measurement of spectrum lines, especially iron lines. In the determination of the wave-length of a line by interpolation between two lines of known wave-length a mean error of approximately 6×10^{-4} Å has been achieved. The method has been improved by a new way of determining the centre of the interference lines. Also an iron hollow-cathode has been tested and adapted for spectrophotometric measurement.

The authors wish to express their gratitude to Professor Erik Hulthén for much good advice and valuable help in the course of the work and to fil. lic. H. Neuhaus, who has been very helpful, especially in connection with the testing of the hollow-cathode.

Review of the main principles

The optical arrangement before the entrance slit of the spectrometer forms two branches (Fig. 1). One of them, the spectrum branch, gives at the focal plane of the spectrometer the spectrum to be investigated. The other one, the interference branch, gives an interference pattern composed of narrow, vertical, parallel lines (Fig. 2). These are obtained by a Fabry-Perot etalon through which passes a parallel beam of white light, and the wave-number difference between two orders is a constant, here 0.25 cm^{-1}. The two patterns, which overlap, are recorded by one photomultiplier. The light of the two branches is modulated with choppers into two different frequencies (spectrum 600 c/s, interference 3900 c/s), and this arrangement facilitates an electronic separation of the two signals from the photomultiplier.

The spectral signal obtained with this separation is amplified and filtered, and it is then recorded with a recording instrument. The interference signal is amplified, rectified and filtered. The D.C. voltage thus obtained releases, when it passes a definite level, a short pulse which is recorded with the same writing tool as records the spectrum. Thus no parallaxes are introduced.

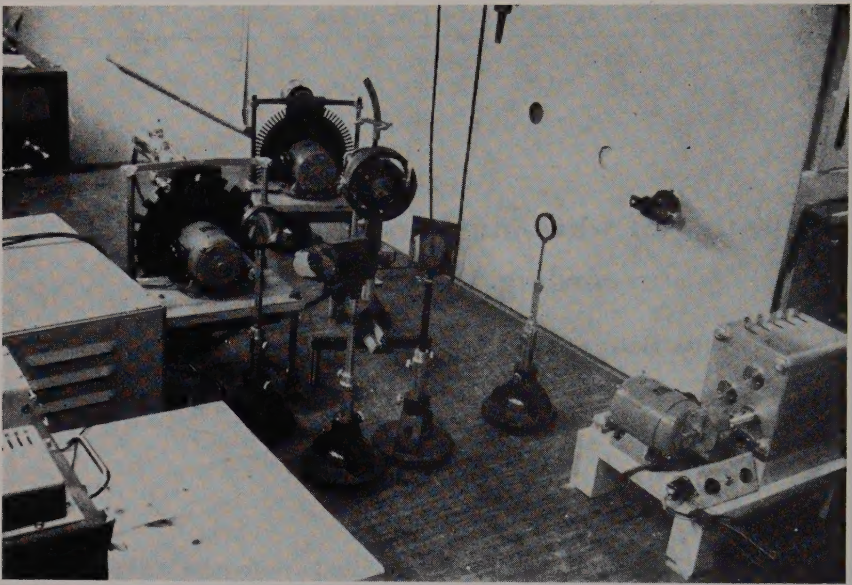

Fig. 1. The optical arrangement. The entrance slit of the spectrometer is on the right, the half-silvered mirror is in the centre and to the left of it there is a right-angled prism, which reflects the light of the spectrum branch through 90°.

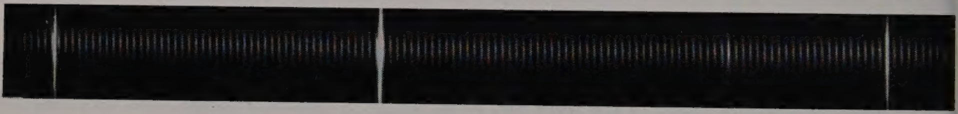

Fig. 2. The interference pattern and some spectral lines.

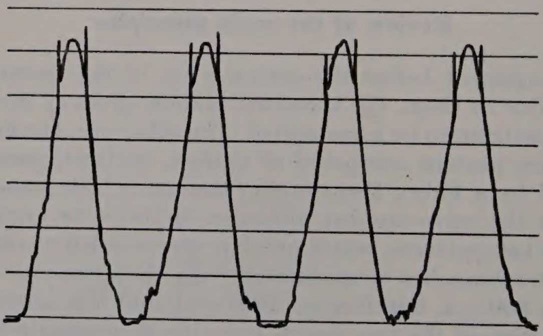

Fig. 3. Interference lines with level indications.

Fig. 3 has been obtained by recording the interference lines with the spectrum amplifier. The corresponding pulses from the interference amplifier have been recorded simultaneously, and the figure shows how the centre of the interference line is defined

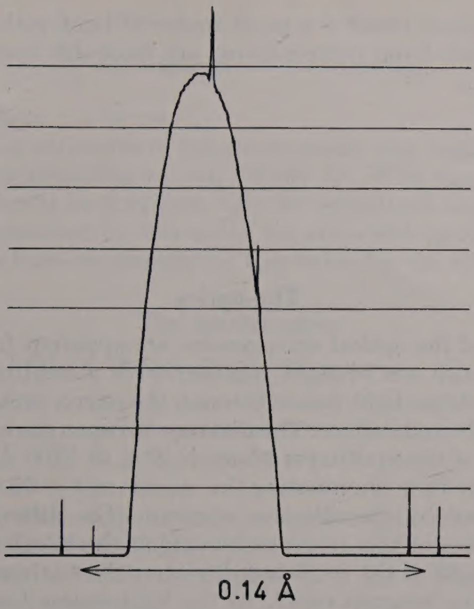

Fig. 4. Spectral line with wave-number marks.

by the two level marks. Fig. 4 shows a recorded spectrum line and the level marks corresponding to three interference lines. The recorded amplitude may be compared with the blackening of a photographic plate, since the amplitude scale of the recorder is logarithmic.

The light sources

General requirements of spectrophotometric recording are good stability and high intensity. With precision measurement a narrow width of the spectrum-line is also desirable. The iron hollow-cathode constructed by H. M. Crosswhite, G. H. Dieke and C. Salmon Legagneur [2] has been found to fulfil these requirements. The hollow-cathode used by the authors differs mainly from this, in that no uranium-getter has been used. Different carrier gases (neon, argon, krypton) and different electrode dimensions have been tested. For the present purpose the following data have been found to fit best:

Carrier gas: neon.
Pressure: 3 mm Hg.
Current: 100 mA with a voltage of 185 V.
Ignition voltage: 220 V.
Anode: Nickel (diameter 19 mm).
Cathode: Swedish iron (length 50 mm, depth 40 mm, outer diameter 9 mm, inner diameter 6 mm).
Distance anode–cathode: 10 mm.

The power for the hollow-cathode has been obtained from a high voltage power supply, well filtered.

The interference branch requires a point-source of light with high colour temperature. A zirconium–oxide lamp (concentrated arc discharge-lamp) with the following data has been used:

Effect, 100 W.
Brightness, 39 candle/mm^2.
Candle-power, 7 candles.
Spot diameter, 1.5 mm.
Colour temperature, 3200°K.

The optics

The chief outlines of the optical arrangement are apparent from Fig. 1. The light-beams from each branch are brought together with a semi-transparent mirror, so arranged that the spectrum-light passes through the mirror and the interference-light is reflected from the silvered surface. The distance between the etalon plates is 20 mm. The reflecting power of the multilayer plates is 92 % at 5200 Å.

The part of the light-flow illuminating the spectrometer slit which can be utilized for recording is limited by the effective aperture. The different lenses have been selected to make full use of this aperture, to exploit the interference-light as fully as possible. The focal length of the condenser-lens must be so chosen that the curvature of the interference lines becomes small. As the light-source has a certain extension, beams making a small angle with the light-normal will also pass through the interferometer. The dispersion of the spectrometer will then give rise to a curvature of the interference lines (convex to longer wave-lengths). It is desirable to utilize the whole length of the interference-lines determined by the spot-diameter of the light-source in order to get the maximal quantity of light to the photomultiplier. For a definite width of the photomultiplier-slit the greatest permitted curvature is then determined from the condition that the whole curved line just fits in the opening of the slit. The curvature depends on the focal length of the condenser-lens and the light-source dimensions, as follows:

For the dispersion of the interferometer it holds that

$$\lambda = \lambda_0 \left(1 - \tfrac{1}{2}\left(\frac{r}{f}\right)^2\right),$$

where

λ_0 = the wave-length at normal incidence,
r = the spot-diameter, and
f = the focal length of the condenser-lens.

There are further introduced

$\frac{\partial l}{\partial \lambda}$ = the linear dispersion of the spectrometer,
Δl = the maximal deviation of the curved line from a vertical straight line through the vertex, and
b = the slit-width of the photometer.

The condition then becomes:

$$|\Delta l| = \tfrac{1}{2}\frac{r^2}{f^2}\lambda_0 \frac{\partial l}{\partial \lambda} < b.$$

Numerically:

$$\lambda_0 \sim 5000 \text{ Å} \qquad r = 1.5 \text{ mm}$$

$$\frac{\partial l}{\partial \lambda} = 2.7 \text{ mm/Å} \qquad b = 0.05 \text{ mm}$$

The condition then gives: $f > 55$ cm.

The optimal entrance slit-width of the spectrometer can be theoretically calculated for non-coherent light according to van Cittert [3]. With the present spectrometer data the slit-width should be 0.02 mm. Our investigations show, however, that the increase in intensity obtained by increasing the slit-width to 0.05 mm well warrants the broadening of the lines accompanying this value for the slit-width.

The spectrometer

The following data hold for the spectrometer:

Grating: Echelle 300.
Mounting: Littrow.
Focal length: 3.5 m.
Dispersion: 2.7 mm/Å at 5400 Å.

Measurements have been undertaken in a wave-length interval at about 5400 Å in the 11th order and at a blaze-angle of 60°.

To avoid overlapping of orders the dispersion of the echelle has been crossed at right angles with that of a prism.

The photometer

The width of the photometer-slit is equal to that of the spectrometer.

The mounting of the photometer is shown in Fig. 5. A microscope can be pushed into the photomultiplier-housing to facilitate focussing and adjustment of the slit.

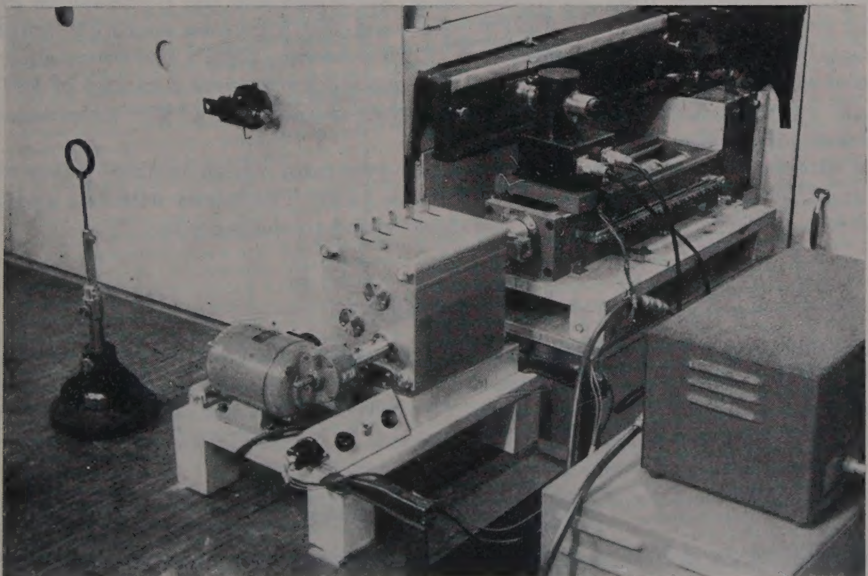

Fig. 5. The photometer arrangement. The photomultiplier-housing is in the upper right-hand corner and the gear-box is in the centre of the picture.

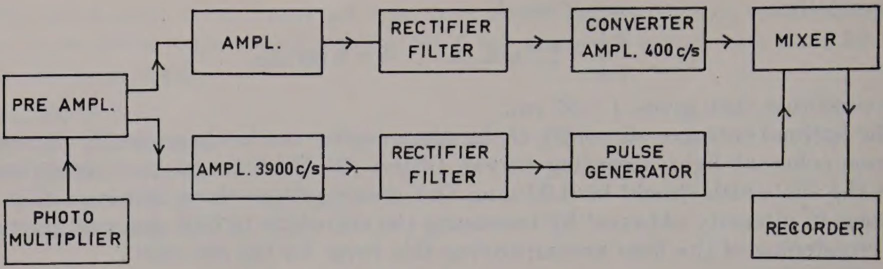

Fig. 6. Block diagram of the electronic equipment.

The multiplier-housing is moved by a comparator screw with a diameter of 40 mm and a pitch of 1 mm. The screw is turned by a synchronous motor via a gear-box. This has 5 gears and covers a gear-range from 1:1 (27 rpm) to 1:100. The photometer automatically changes direction at the end-points of an adjustable interval.

The electronic equipment

The electronic equipment appears from the block diagram in Fig. 6. The signal from the multiplier is fed to the pre-amplifier mounted close to the latter. The pre-amplifier consists of two amplifiers tuned to the two modulation frequencies. From here the signals are fed to the spectrum amplifier and the interference amplifier. Both of these incorporate arrangements for the rectifying and filtering of the signals. The filtering is needed to increase the signal-to-noise ratio. By rectifying the signal before it enters the filters a simple low-pass filter with easily variable time-constant may be used. A band-pass filter would not be so suitable since the fluctuations of the carrier frequencies set a lower limit to the band-width. In the spectrum amplifier the signal must again be converted to A.C. after having passed the filter, since the recorder must be fed with A.C. voltage. A converter introduces a carrier of 400 c/s. Also the spectrum amplifier incorporates another amplifier stage this latter tuned to the converter frequency.

The interference amplifier contains a pulse-generator which releases pulses when the input voltage passes a certain level. These pulses are mixed with the spectrum signal in a mixer. From the mixer the signal is fed to the recorder.

The pre-amplifier

Circuit diagram in Fig. 7. The input-stage common to the two branches is a cathode-follower. Each branch forms a staggered tuned-pair, the amplification of each branch equals 2000 and $Q \sim 20$ for each stage. The output-stages are cathode-followers, to match low-impedance cables.

The spectrum amplifier

Circuit diagram in Fig. 8. A good linearity within an amplitude range of 25 dB, the range of the recorder used, is required of the spectrum amplifier. This linearity has been achieved by applying negative feedback to the amplifier stages preceding

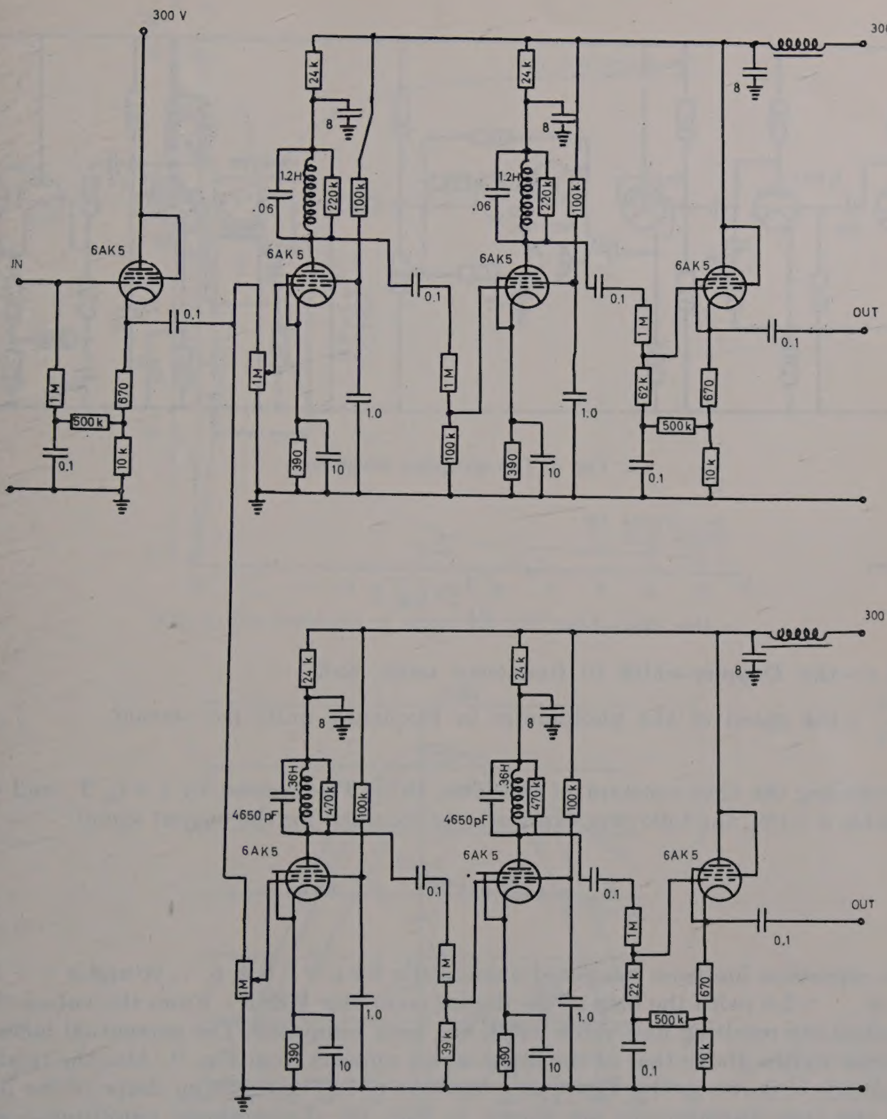

Fig. 7. The pre-amplifier.

the rectifier. The bad linearity of the rectifier at low signal-levels is not significant as all levels below 1 V from the rectifier-output are cut out. Further on, the filter must introduce only negligible distortion of the line shape. The outlay of the filter is based on the following theoretical considerations [4]:

The signal is supposed to be Gauss-shaped, that is

$$E_{\text{in}} = e^{-(t/t_0)^2}$$

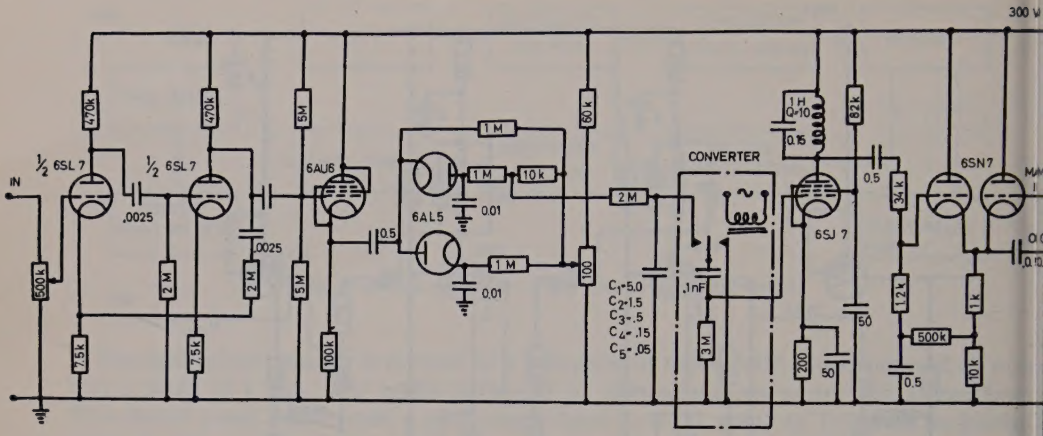

Fig. 8. The spectrum amplifier.

where

$$t_0 = \frac{\Delta \sigma}{\dfrac{\partial \sigma}{\partial t} 2 \sqrt{\log 2}},$$

$\Delta \sigma$ = the Doppler-width in frequency units, and

$\dfrac{\partial \sigma}{\partial t}$ = the speed of the photometer in frequency units per second.

Introducing the time-constant of the filter RC $= T$ expressed by $\varepsilon = t_0/T$, and the variable $x = t/t_0$, the following expression is obtained for the output signal:

$$E_{\text{out}} = \varepsilon\, e^{\varepsilon^2/4}\, e^{-\varepsilon x} \int_{-\infty}^{x-\varepsilon/2} e^{-v^2}\, dv.$$

This expression has been computed numerically for $\varepsilon = 1, 3.4, 5, 7, 10$ and $x = -2.0, -1.9 \ldots +2.0$ (with the help of the digital computer BESK). From the values thus obtained the resulting half-value width has been computed. The percentual increase of these widths above that of the input-signal appears from Fig. 9. Also the relative amplitude is shown in this figure as a function of ε. The resulting shape of the lines and the time-displacement are shown in Fig. 10. (Logarithmic amplitude-scale.) From these theoretical curves it has been concluded that if ε is approx. 5, the resulting distorsion is negligible as compared with other sources of error. Fig. 11 shows experimental recording corresponding to the values of the parameter in Fig. 10.

The interference amplifier

Circuit diagram in Figure 12. In the interference amplifier the distortion of the line-shape caused by inlinearity and by the filter is of minor importance, since the output-signal after steady-state has been reached will in any case consist of similar

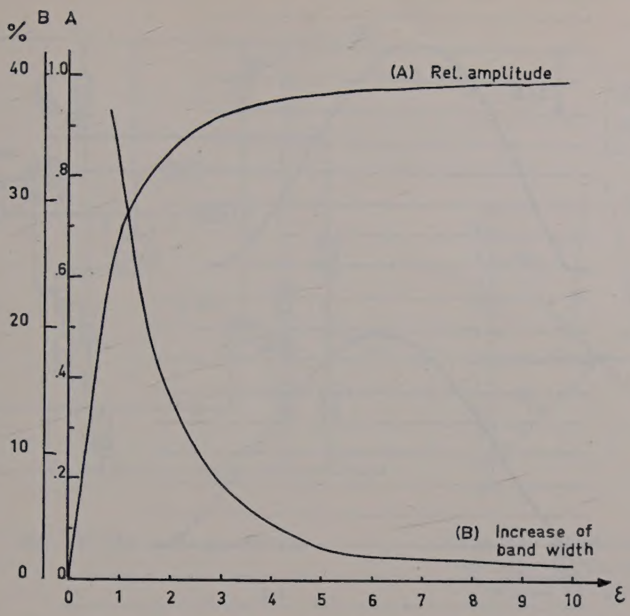

Fig. 9. The variation of amplitude and band-width with ε.

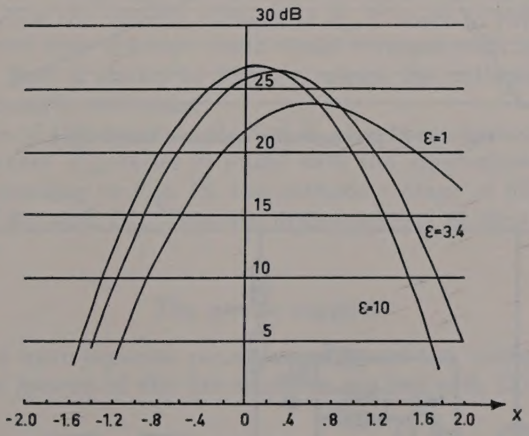

Fig. 10. Theoretically estimated line-shapes.

signals at equal intervals. The amplifier and the filter have, however, been so dimensioned and tested that the distortion is comparatively small, as shown in Figure 3.

The pulse-generator

Circuit diagram in Fig. 13. The principle of the pulse-generator is based upon the features of the gated-beam pentode 6BN6. The anode current of this tube is zero if

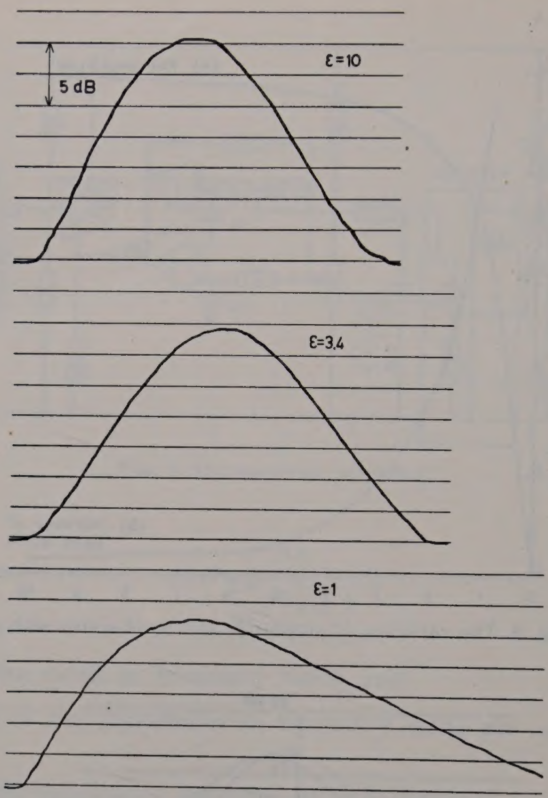

Fig. 11. Experimentally obtained line-shapes.

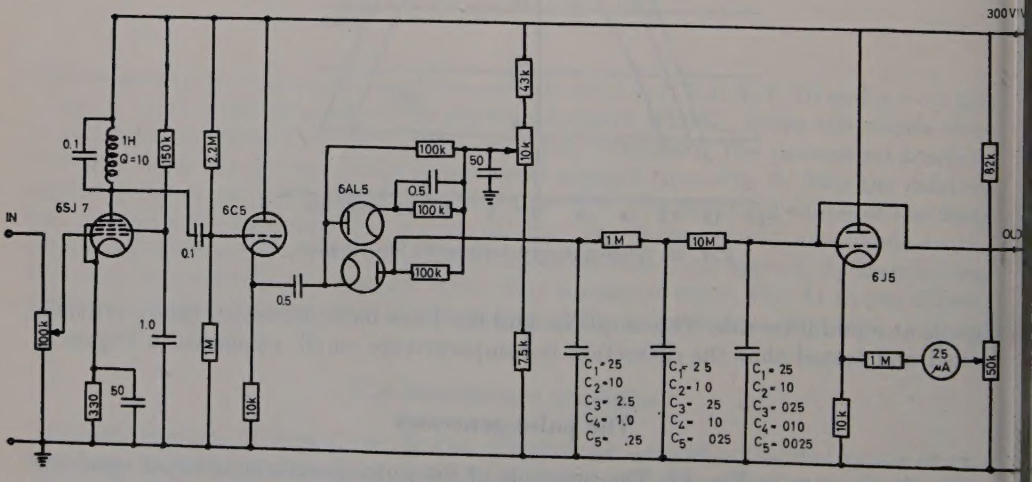

Fig. 12. The interference amplifier.

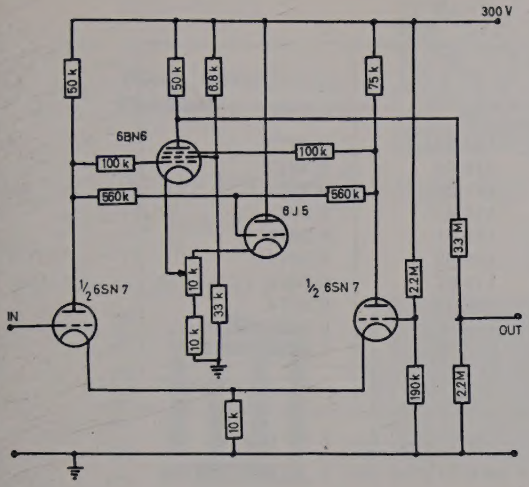

Fig. 13. The pulse-generator.

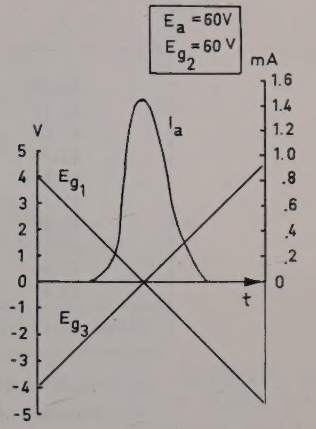

Fig. 14. Anode current of the pentode 6BN6, $E_{g\,1}$ and $E_{g\,3}$ varying in opposite phase.

either the control grid voltage E_{g1} or the suppressor grid (second control grid) voltage E_{g3} is some volts below the cathode voltage. If E_{g1} is made to vary in opposite phase to E_{g3}, the tube will only conduct when these voltages both approximate to the cathode potential. This is shown in Fig. 14, where the voltages E_{g1} and E_{g3} are supposed to vary linearly with time.

A phase difference of 180° between E_{g1} and E_{g3} has been obtained with a difference-amplifier circuit, where E_{g3} varies in phase with the input-signal. With a cathode-follower circuit, according to Fig. 13, the cathode voltage of 6BN6 will always be about the mean of E_{g1} and E_{g3}. Thus the drift tendency of the circuit is essentially eliminated.

The power supplies

All the amplifiers have separate power supplies and the voltages are well filtered and stabilized. The heaters of the pre-amplifier are fed with D.C. current to avoid hum.

Measurements and results

To investigate the requirements of accuracy met with the method, measurements have been undertaken on three lines in an interval of about 8.7 Å. In Table 1 are presented the results of a series of measurements of 10 recordings.

According to Edlén [5] the wave-lengths of the lines are:

1. 5397.1311 Å = 18528.362 cm^{-1} Fe
2. 5400.5617 Å = 18516.593 cm^{-1} Ne
3. 5405.7781 Å = 18498.725 cm^{-1} Fe

Table 1.

n_x	n	n_x/n
47.08	118.46	0.3975
47.11	118.59	0.3972
47.08	118.58	0.3971
47.08	118.60	0.3970
47.10	118.61	0.3971
47.13	118.69	0.3971
47.12	118.67	0.3970
47.13	118.59	0.3974
47.30	118.96	0.3976
47.97	118.25	0.3976
Mean 47.11 ± 0.03	118.60 ± 0.06	0.39722 ± 0.00007

n_x = number of wave-marks from line 1 to line 2.
n = number of wave-marks from line 1 to line 3.

The value of the mean error of n_x/n corresponds to an error of 0.0006 Å.

Since the mean errors of n_x and n are large compared to the error of n_x/n, it may be presumed that fluctuations appear in the interferometer from one recording t another. From this one may assume that the errors may be diminished if the interferometer is protected against temperature and pressure fluctuations, which may also exert an influence during one and the same recording.

Physics Department, University of Stockholm, April 1956.

REFERENCES

1. B. Å. Krantz and N. Åslund, Arkiv för Fysik *10*, 165 (1955).
2. H. M. Crosswhite, G. H. Dieke, and C. Salmon Legagneur, J. Opt. Soc. Am. *45*, 271 (1955).
3. P. H. van Cittert, Z. Phys. *65*, 257 (1930); Z. Phys. *69*, 298 (1931).
4. S. Brodersen, J. Opt. Soc. Am. *43*, 1216 (1953).
5. Commission des étalons de longeur d'onde et des tables des spectres.

Tryckt den 7 februari 1957

Uppsala 1957. Almqvist & Wiksells Boktryckeri AB